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Parallel β-sheet assemblies at interfaces

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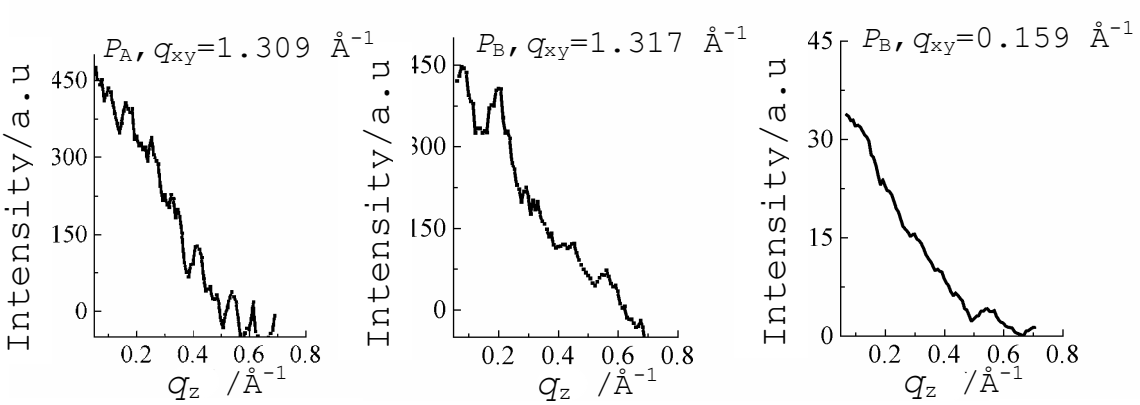
1. GIXD experimental

GIXD experiments were performed with the liquid surface diffractometer at the undulator BW1 beam line at the HASYLAB synchrotron source (Hamburg, Germany). The peptide films were spread at room temperature and diffraction measurements were performed at 5°C. A monochromatic X-ray beam was adjusted to strike the liquid surface at an incident angle ($a \approx 0.85ac$ where ac is the critical angle for total external reflection) which maximizes surface sensitivity. The dimensions of the footprint of the incoming X-ray beam on the liquid surface were approximately 2 by 50 mm. GIXD signals were obtained from two-dimensional crystallites randomly oriented about the water surface normal. The scattered intensity was collected by means of a position-sensitive detector (PSD) which intercepts photons over the range $0.0 \leq q_z \leq 1.3$ Å^{-1}, q_z being the out of plane component of the scattering vector. Measurements were performed by scanning the horizontal component, $q_{xy} \approx 4\pi \sin \theta_{xy} / \lambda$, of the scattering vector, where $2\theta_{xy}$ is the angle between the

incident and diffracted beam projected onto the horizontal plane. The diffraction data are represented in two ways: (1) The GIXD pattern $I(q_{xy})$, obtained by integrating over the whole q_z window of the PSD, shows Bragg peaks; (2) Bragg rod intensity profiles are the scattered intensities $I(q_z)$ recorded in channels along the PSD but integrated across the q_{xy} range of each Bragg peak. The q_{xy} positions of the Bragg peaks yield the lattice spacings $d = 2\pi / q_{xy}$, which may be indexed by the two Miller indices h,k to yield the unit cell. The full width at half maximum (FWHM(q_{xy})) of the Bragg peaks yields the lateral 2D crystalline coherence length $L_{xy} \approx 0.9(2\pi) / \mathrm{FWHM}(q_{xy})$. The width of the Bragg rod profile along q_z gives a first estimate of the thickness of the crystalline film: $L_z \approx 0.9(2\pi) / \mathrm{FWHM}(q_z)$. The diffraction data are represented either as the measured intensities or after correction for the Lorenz-polarization and active area (LPA) factors. Bragg peak intensities for the proposed models can be roughly evaluated using the CERIUS[2] computational package (Accelrys, Paris).

2. Bragg rods

Bragg rods of P_A and P_B ordered films. According to the FWHM(q_z), the films are 11.5, 12.4 and 11.5 Å thick respectively, i.e., of monolayer thickness.



3. The P_AP_B subcell (not to scale) that provides reasoning for the 4.18 Å spacing. The cell is constructed based on the reasonable assumption that the distance between every other amino acid is 6.9 Å, and on the observed values of 4.76 and 4.18 Å. Ellipses represent phenyl rings expected to enhance the diffraction corresponding to the (1,-1) spacing.